Abstract Submitted to the
International Conference on Strongly Correlated Electron Systems
University of Michigan, Ann Arbor
August 6-10, 2001

Superexchange in transition metal oxides: new examples

V. Yushankhai, L. Siurakshina
Max-Plank-Institute for the Physics of Complex Systems, D-01187, Dresden, Germany
and Joint Institute for Nuclear Research, 141980 Dubna, Russia

Recently various types of interplay between magnetic, charge, and orbital degrees of freedom have been newly found and re-examined for the fast growing family of transition metal (TM) oxides. This interplay raises new challenging problems in the theoretical description of new TM oxides. In particular, the standard concepts of the superexchange theory are not sufficient to derive effective quantum spin models required to explain a rich variety of magnetic properties of new materials. We develop further and apply these concepts to the following particular compounds and problems.
(1)Anisotropic superexchange in the cuprate compound $Ba_3Cu_2O_4Cl_2$ which contains the elementary Cu–O_2–Cu magnetic bonds arranged into strongly folded chains. Special attention is payed to the derivation and subsequent analysis of the form for the symmetric anisotropy in this material.
(2)Variation of the exchange integrals in the quarter-filled two-leg ladder system NaV_2O_5 under the phase transition into a charge ordered state. Not only the intra-ladder spin-spin coupling, but the inter-ladder superexchange is considered in details as well.
(3)The concept of interference of different superexhange pathes, the so-called ring exchange, is re-examined and discussed on a general background.
In all cases the derivation is based on a perturbation expansion of generic multiorbital Hubbard Hamiltonians.